

## Workshop EIG-Concert

Scientific Program (September 14, 2021)

9:20 – Valentin Valtchev – Opening

9:30 – 10:00 – Remy Guillet-Nicolas - Advanced Porous and Textural Engineering of Zeolitic Materials for a Cleaner Energy

10:00 – 10:30 – El Hassane LAHRAR – Cation-exchange forms analysis of CHA-type zeolite

**10:30 – 10:50 Coffee break**

10:50 – 11:20 – Eddy Dib - Local order in zeolites: An alliance of NMR and DFT

11:20 – 11:50 – Ahmed Omran – Gas hydrates: Properties and opportunities

**12:00 – 14:00 Lunch**

14:00 – 14:30 - Y. Kubota - Structure particularities of YNU-5 (YFI) and YNU-2 (MSE)

14:30 – 15:00 - P. St. Petkov - *Ab initio* molecular dynamic simulations of silicon migration towards silanol nest in MSE type zeolite

Authors: P. St. Petkov, K. Simeonova, I. Z. Koleva, H. A. Aleksandrov, G. N. Vayssilov

15:00 – 15:30- G. N. Vayssilov - Theoretical study of titanium, aluminum, and vacancies in tetrahedral positions of MSE-type zeolite framework

Authors: P. St. Petkov, K. Simeonova, I. Z. Koleva, H. A. Aleksandrov, G. N. Vayssilov

15:30 – 16:00 - K. Simeonova - Discussion on Computational modeling of YNU-5 zeolite: preliminary results and probable concepts.

Authors: K. Simeonova, P. St. Petkov, G. Vayssilov

**16:00 – 16:20 Coffee break**

16:20 – 18:00 Open discussion